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Local atomic order in apparently disordered crystals: What we can learn from Pair Distribution Function. Radovan Černý^a, Yaroslav Filinchuk^b, Joanna Ropka^a, Yiyang Li^c. ^aLab. of Crystallography, Univ. of Geneva, Switzerland. ^bSwiss-Norwegian Beamline at ESRF, Grenoble, France. ^cInst. of Appl. Phys., Univ. of Sci. Tech., Beijing, China.
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Many metallic alloys, intermetallic compounds and metal hydrides show disordered crystal structure (partly or mixed occupied and/or split or close atomic sites) when Bragg scattering is analyzed by the Rietveld method. If the crystal appears from Bragg scattering as disordered, it does not mean that it cannot be ordered locally. Significant, and often sufficient, information about the local order can be gleaned from the analysis of the atomic Pair Distribution Function (PDF) obtained from the Total Scattering which samples Bragg and diffuse scattering data of a polycrystalline sample simultaneously. The local ordering in apparently disordered crystal is of high importance in determining the materials property, and helps to understand the chemical bonding in the crystal. We will show on two examples what is possible to learn from the PDF obtained from a powder sample:

The crystal structure of YCu_{6.576}, a substitution variant of the CaCu₅-type, was shown to contain Cu₂-dumbbells replacing Y-atoms in a fraction $s=0.19$ in the formula Y_{1-s}Cu_{5+2s}. The structure type TbCu₇ is assigned to the disordered structure. The local order in the vicinity of the Cu₂-dumbbells has been derived from the PDF obtained from the X-ray powder data [1]. The coordinating Cu₆-hexagon around the dumbbell site shows a shrinkage of 0.33(1) Å *w.r.t.* the equivalent environment of the Y-atom. No adjacent Y-atoms are substituted but a hexagonal arrangement of Cu₂-dumbbells exists in layers perpendicular to *c*. The stacking along [001] is random and can be modeled locally from the PDF data consistent with both *ab*- and *abc*-type stacking. Therefore, the local order is comparable to that in Ni₁₇Th₂- and Th₂Zn₁₇-structure types, ordered variants of TbCu₇. These results agree with the recent atomistic simulations based on interatomic pair potentials extracted from *ab-initio* calculated total energy curves by adopting modified Möbius inversion method [2].

Deuterium local order in cubic Laves phase deuteride YFe₂D_{4.2} was studied by neutron (*ToF*) powder diffraction experiments and PDF modeling [3]. The minimal D-D distance in a metal hydride of 2.1 Å (Switendick rule) has been experimentally proved in the HT-disordered phase. The distribution of deuterium atoms around the iron is not random, and cannot be explained only by applying the Switendick rule. The local order of deuterium atoms within the first iron coordination sphere in the HT-disordered phase above 343 K is similar to the iron coordination in the LT-ordered phase. Same composition of the coordination polyhedra FeD₅ and FeD₄ was found in both phases by Reversed Monte Carlo modeling of the PDF. The exact shape of the FeD₅ and FeD₄ coordination polyhedra in the HT-disordered phase cannot be, however, unambiguously revealed by the PDF analysis.

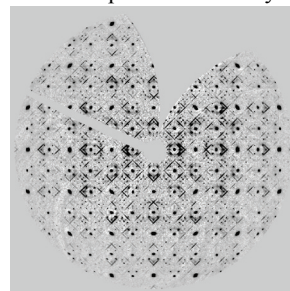
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α-“NaLuF₄” : A crystal with Twinning, Modulation and Diffuse Scattering. Partha P. Das^a, Lukas Palatinus^b, Hans-Beat Bürgi^{a,c}, Anthony Linden^a. ^aInst. of Organic Chemistry, University of Zürich, Switzerland. ^bDepartment of Structure Analysis, Prague, Czech Republic. ^cDept. Chemistry and Biochemistry, University of Bern, Switzerland.
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NaLnF₄ (Ln=Y, La-Lu) crystallizes in two predominant forms. The low temperature, stable hexagonal β-form, doped with various Ln³⁺ ions shows efficient light upconversion properties. Understanding these properties requires a knowledge of the local structure; the average structure of β-NaLaF₄ has occupational disorder within columns of mixed Na⁺/La³⁺ sites and Na⁺/vacancies; an examination of strong diffuse scattering allowed the relative alignments of the columns to be deduced [1]. We are studying the structure of α-NaLuF₄ (high temperature phase) with likely composition Na₅Lu₉F₃₂, and have recorded the full scattering using synchrotron radiation. Reconstructed reciprocal lattice layers reveal a rich, apparently cubic diffraction pattern with very strong main reflections, weaker satellites and strong diffuse scattering. Stronger main reflections in reciprocal lattice rows are not collinear and at higher angles splitting of these reflections were observed. Therefore, the highest possible symmetry is tetragonal and 6-fold twinning accounts for the apparent cubic symmetry. If the satellites are treated as Bragg peaks, one can derive an orthorhombic cell with space group *Cmmm*. The structure could be solved in the 5-fold supercell using Superflip^[2] which reveals two distinct commensurately modulated parallel columns of cations: one with varying Na⁺/La³⁺ occupancy and one with positional displacements of the ions from the average structure positions.



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Diffuse x-ray scattering from correlated dislocations in epitaxial layers. Vaclav Holy. Charles University in Prague, Czech Republic.
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Diffuse x-ray scattering from straight misfit and threading dislocations in epitaxial layers has been simulated using numerical Monte-Carlo method, which makes it possible to include a correlation of dislocation positions. The simulations yielded reciprocal-space distributions of diffusely scattered intensity both in coplanar and non-coplanar scattering geometry (grazing-incidence diffraction). From the results it